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MEETING ON THE PHYSICS OF TRANSITION METALS LEEDS, UK, 18-22 AU--ETC(U)
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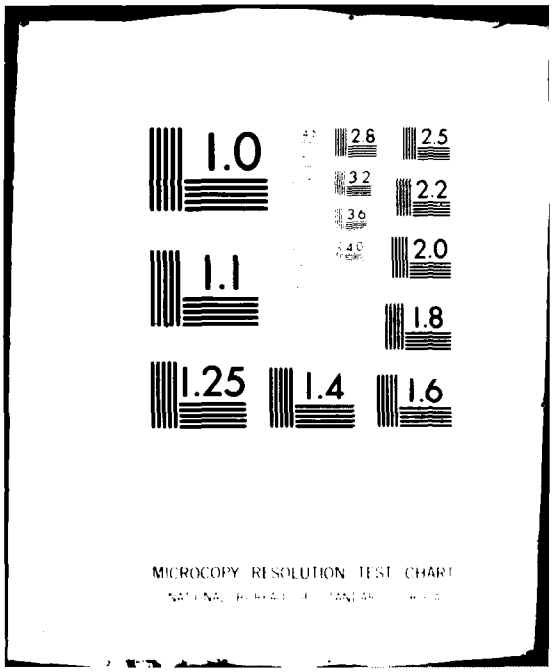
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MEETING ON THE PHYSICS OF TRANSITION METALS
LEEDS, UK, 18-22 AUGUST 1980.

JOHN R. NEIGHBOURS FOR DIMITRIS PAPACONSTANTOPOULOS AND BARRY KLEIN

30 OCT 1980

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

This report covers the conference on transition metals held in Leeds on 18-22 August 1980. Subjects covered were band theory, ferromagnetism, ultrasonic attenuation, neutron scattering, magnetism, Fermi surfaces, positron annihilation, lattice dynamics and heats of formation. The meeting included 25 papers, 4 poster sessions and a panel discussion on magnetism in metals.

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MEETING ON THE PHYSICS OF TRANSITION METALS
LEEDS, UK, 18-22 AUGUST 1980

The International Conference on Physics of Transition Metals was held at the University of Leeds, UK, from 18-22 August 1980. Over 200 scientists, primarily from Europe and North America, participated in this successor to the 1977 Toronto meeting on the same topic. The conference was organized into 29 invited papers and over 100 contributed poster talks, with the former divided approximately evenly between lectures on magnetism and nonmagnetism. An additional highlight of the meeting was the awarding of the European Physical Society Solid-State Physics Prize jointly to O.K. Anderson and A.R. Miedema for their work on band structure techniques and applications, and empirical models and energy effects in alloys, respectively. It was widely felt that this was a highly successful meeting, with a great deal of "interaction" between the participants. Particularly well-done was the poster session scheduling, with several free hours every afternoon devoted solely to the posters.

E.P. Wohlfarth (Imperial College) gave the introductory lecture of the conference on the history of the Stoner theory of itinerant electron ferromagnetism. This theory is based on a band model, Fermi statistics, and a mean field to represent magnetic interactions. He discussed applications to real materials, both strong and weak itinerant ferromagnets, a unification of the Landau-Ginzburg formalism and certain controversial issues which led to a panel discussion later on in the conference.

J. Callaway (Louisiana State Univ.) reviewed recent band structure calculations for ferromagnetic transition metals and compared them with experimental results. He pointed out the good agreement between theory and experiment for the hyperfine field, the magneton number, and to some extent for the Fermi surface. However, serious discrepancies occur between theory and measurements of angle-resolved photoemission for nickel. This seems to be a problem which receives a lot of attention but with no consensus yet for an explanation. Calloway also emphasized the importance of performing reliable band calculation for cobalt which may shed some light in understanding the Ni anomaly.

E. Fawcett et al (Univ. of Toronto) talked about measurements of the attenuation of ultrasound in antiferromagnetic chromium as a function of magnetic field. These measurements show two phase transitions with the lower field and the lower temperature transition terminating at a critical end-point.

Y. Ishikawa (Tohoku Univ.) presented neutron scattering studies of magnetic transition metals and alloys. He opined that in a localized spin system the magnetic properties at finite temperature are explained by the Heisenberg theory and the magnetic excitations at the lowest temperature are consistent with the energy band calculations. Ishikawa also reported observations of the excitations in the Stoner continuum. Above the Curie temperature the low energy excitations of the Moriya spin fluctuations theory are present.

The muon spin rotation (μSR) technique for an interstitial positive muon in a ferromagnetic host was discussed by B.D. Patterson (Univ. of Zurich). This technique is based on the phenomenon that a muon undergoes Larmor precession at a frequency determined by the local magnetic field at the muon site. Information about the motion of the muon is provided by the linewidth of the μSR signal. The results indicate that the light muon, in contrast to the heavier hydrogen isotopes, moves through the iron lattice via coherent quantum tunneling.

R. Zeller (Inst. für FestKörperforschung, Julich) told of his calculations of the electronic structure of transition metal impurities in ferromagnetic Ni. Zeller uses a Green's function method and treats exchange and correlation in the local spin density approximation. The calculations show that the impurities have either ferromagnetic or antiferromagnetic local moments. This is a first principles theory which gives reasonable agreement with experiment.

Some results from the Netherlands were reported by P.E. Brommer (Univ. of Amsterdam) and H. van Dongen (Kamerlingh Onnes Laboratory). Brommer reported susceptibility and specific heat measurements on a series of non-stoichiometric compounds of the type $TiFe_xCo_{1-x}$. These quantities vary strongly as a function of concentration x which suggests that the magnetic properties of ordered alloys appear to be strongly influenced by structural defects. van Dongen presented measurements of susceptibility, magnetization, electrical resistivity and Mössbauer spectra for pseudobinary Laves phase compounds of the form $Y(Co_{1-x}Fe_x)_2$, $Y(Ir_{1-x}Fe_x)_2$ and $Hf(Co_{1-x}Fe_x)_2$. For $Y(Co_{1-x}Fe_x)_2$ the low field ac susceptibility exhibits spin-glass-like peaks. For $Y(Ir_{1-x}Fe_x)_2$, for $x < 0.4$, the electrical resistivity decreases with increasing temperature. Magnetization measurements show magnetic ordering at different concentrations for each alloy. The results suggest the possibility of studying magnetic moment formation, i.e., Kondo effect and the interactions present in spin glasses.

D.E. Eastman (IBM) described how accurate energy band dispersions, E(k), can be determined using angle-resolved photoemission with polarized synchrotron radiation. He described the experimental equipment used on the Wisconsin synchrotron, and also a number of recent results. The latter included studies of experimental band dispersions and their trends for: (1) 3d bands in Cr, Fe, Co, Ni, Cu, and Zn; (b) 4d and 5d bands in Pd, Ir, Pt, and Au; (3) measurements of the k-dependent magnetic exchange splittings for Fe, Co, and Ni. Although the experimental and theoretical energy bands generally are in fairly good agreement, there are notable exceptions (Ni is a good example). Keeping in mind that the photoemission experiment measures an excited state of the solid system, it is not surprising that there is some disagreement with the ground state one-electron (Koopman's) energies. There was extensive discussion regarding this point with the conclusion that the problem needs further looking into.

H. Hasegawa (Univ. of Tokyo) proposed a finite-temperature band theory in which effects of local spin fluctuations are taken into account by means

of the static functional integral method combined with the single-site analogy approximation. The theory seems to give a satisfactory picture of finite temperature properties of iron and nickel.

V. Korenman (Univ. of Maryland) presented the Korenman-Prange local-band theory of itinerant electron ferromagnetism which has the special feature that the exchange potential is related to the local magnetization rather than the mean magnetization. As a result, spin-split bands may be maintained above the Curie temperature and so there need be no strong electron anomalies at the critical temperature, T_c. The theory shows that nickel and iron have short-range magnetic order even above T_c. Korenman showed calculations of the magnon spectrum which were in good agreement with experiment. Also this theory was able to explain localized behavior at high temperatures.

Calculations by B.S. Shastry, D.M. Edwards and A.P. Young (Imperial College) on the static and dynamic properties of an effective Heisenberg model of iron were reported by Shastry who claimed that their calculated neutron scattering function is compatible with the experimental data of J.W. Lynn (Univ. of Maryland). This was disputed by Lynn himself who emphasized that his data shows a well-defined spin wave peak above T_c, while Shastry's calculations do not. The existence of such spin waves is central to the bases of the Korenman-Prange theory, and this point was discussed at length.

In a session on electrons in metals, B.L. Gyorffy (Univ. of Bristol, UK) lectured on the theory of transition-metal random alloys which has been developed by the Bristol group in collaboration with theoreticians at Oak Ridge National Laboratory. Energy bands of alloys such as Cu-Ni or Pd-Ag have been calculated using the KKR-CPA method, and Gyorffy showed that it was still possible to define a Fermi surface for the alloy even though the E(k) was a complex quantity (k is not a "good" quantum number in the random alloy). This is because the Bloch spectral function still has well-defined peaks (though not delta functions) in the alloy. Gyorffy showed how the KKR-CPA results could be used to calculate electron momentum and two-photon momentum distribution functions relevant to interpreting the Compton profile and positron annihilation (2-d ACAR) experiments. This field appears to have a very promising future.

Recent years have seen the development of several high efficiency 2-d angular correlation spectrometers whose spectra provide visually direct and striking pictures of electronic structure and in particular the Fermi surfaces of metals and alloys. R.N. West (Univ. of East Anglia, UK) described and illustrated the present state-of-the-art of this field, showing spectra for several transition metals and alloys (e.g. Au, Al, V_3Si), and discussing the need for further complementary theoretical work. West emphasized how the phenomenon of low energy positron annihilation in solids yields detailed and illuminating information on electron momentum distributions and Bloch wave vector densities.

In the last paper, G.W. Crabtree (Argonne National Laborartory) discussed the information that can be obtained from de Haas-van Alphen (dHVA)

measurements on transition metals and inter-metallic compounds. With the advent of higher magnetic fields, the ability to reach lower temperatures, on-line Fourier transform techniques and sophisticated parametrization schemes of the band structure, the dHVA method has become a substantially more powerful tool for the study of electronic properties of metals. Crabtree showed how the Fermi surface measurements provide a sensitive test of one-electron theory predictions, while the cyclotron masses can be used to study the many body electron-phonon and electron-electron interactions responsible for superconductivity and magnetism. He reviewed the experimental techniques and the parametrization methods used with illustrative results for Nb, Pt, and Pd, discussed the status of measurements for intermetallic compounds (e.g. Nb_3Sb), and mentioned some promising new directions.

Ordered structures in fcc binary transition metal alloys were discussed by F. Gautier (LMSES, Strasbourg, France). The French group is studying ordering effects within the framework of a generalized perturbation theory starting from the completely disordered state described by a CPA Hamiltonian. They define effective pair interactions (EPI) which vary strongly with concentration and even change sign, and show how the pair correlations depend on band filling and the degree of diagonal and off-diagonal disorder. The range of ordered structures occurring on an fcc lattice was discussed in terms of the EPI.

A.T. Van Kessel (Univ. of Nijmegen, Netherlands) discussed APW (Augmented plane wave) calculations of the Fermi surface of the Nb_3Sb and compared the results with recent dHVA measurements. The agreement between theory and experiment was surprisingly good, especially since the Nijmegen calculations were non-self-consistent. However, it was noted that good quantitative agreement between theory and experiment was obtained only after a k-dependent adjustment of the Fermi energy to optimize the theoretical fit.

Recent advances made in theoretical studies of the electron-phonon interaction dependent properties in transition metals and their compounds were reviewed by W.H. Butler (Oak Ridge National Laboratory). He presented calculations of resistivities, electron-phonon mass enhancements, spectral functions, and phonon linewidths, and noted that regarding agreement with experiment the calculations are generally "astonishingly good" despite what would appear to be drastic approximations used in the theory. Some suggestions on how to improve the calculations (e.g. removing the rigid muffin-tin approximation) were made by Butler who also offered five empirical rules for "finding" high T_c superconductors. These are (1) have a half-filled d-band; (2) make use of Matthias" e/a rules; (3) "rule of togetherness" (high pressure raises T_c); (4) 4d's have higher T_c's than 3d's; (5) rule of the perversity of nature — the high T_c materials are hard to make.

W. Weber (Institut für Angewandte Kernphysic, Karlsruhe) described a microscopic theory of lattice dynamics, developed in collaboration with C. Varma of Bell Telephone Laboratory, especially suited for transition metals and their compounds. The theory is based on a nonorthogonal-tight-binding scheme and employs the idea that the atomic orbitals are moving with the

atomic cores. Weber showed results for NbC, VN , and NbN which reproduced all of the observed anomalous features in their phonon dispersion curves and emphasized that the anomalies could be traced back to special topological features of the electronic energy bands near the Fermi energies, giving large electron-phonon coupling at selected wave vectors. Weber also mentioned that in compounds, hybridization effects additionally enhance the coupling. Finally he showed why high T_c and phonon anomalies seem to occur together: both phenomena are related to the Fermi surface topology and wave functions.

D.G. Pettifor (Imperial College, UK) lectured on his theoretical work regarding heats of formation (ΔH) of transition metal alloys. He derived simple expressions for ΔH using a tight binding approximation with numerical results agreeing with A.R. Miedema's (Phillips Res., Eindhoven) values but differing radically in the physical interpretation. In Miedema's model the attractive term is essentially ionic and arises from the flow of charge between atoms, while in Pettifor's scheme it is covalent in origin, arising from a change in bonding of the localized d-electrons. In addition Pettifor claims that his theory has been verified by the recent band structure calculations of the IBM group (discussed by C.D. Gelatt). In the discussion, Miedema expressed the counter opinion that his model is much more general than Pettifor's, covering a wide range of alloys quite well. Future work will undoubtedly answer these questions.

In a lecture of his own, Miedema applied his approach to studies of heats of adsorption of metals on transition metal substrates. He expressed the enthalpy of adsorption of a metal atom A to a metallic substrate B in terms of the molar surface area of A atoms, the zero temperature surface energies of solid A and B metal, and the heat of solution of A in B. He presented many numerical results.

S. Louie (Univ. of California, Berkeley) discussed electronic structure calculations of d-band metal surfaces and adsorption systems performed using a self-consistent pseudopotential approach. The first-calculations which he reported gave good results for work functions, surface states, adsorbate states and the chemical bonding. For clean surfaces, new surface states are crucial for understanding the spectroscopic measurements. Louie discussed his studies of hydrogen chemisorption on transition metal surfaces, using H on Pd(111) surface as a prototype. In this system, he found that the H atoms prefer to bond onto a 3-fold site over the top site with a strong bonding between the H 1s orbital and the Pd d-states. The calculations are in excellent agreement with experiment.

H.J. Guntherodt (Univ. of Basel, Switzerland) gave an exciting lecture on the subject of metallic glasses, emphasizing the interesting and incompletely understood properties of transition metals and their alloys in the non-crystalline state. These metallic glasses often show negative temperature coefficients of electrical resistivity and positive Hall coefficients. Recent XPS and UPS measurements and some band structure calculations are helping to unravel some of the mysteries of these materials.

B. Stritzker (Inst. für Festkörperforschung, Julich) reported results of superconductivity in irradiated palladium, with T_c values of up to 3.2K using He^+ for the irradiation. Careful studies have led Stritzker to rule out impurity effects as the cause of superconductivity, but he rather feels that the He^+ bombardment creates Pd interstitials. This disordering probably lowers the density of states at E_f and results in a suppression of the spin fluctuations which kills superconductivity in pure Pd. Other possible T_c enhancing mechanisms could be the introduction of soft phonon modes in the disordered Pd.

C.D. Gelatt (IBM) discussed calculations he has done with A.R. Williams and V.L. Moruzzi on bonding in AB compounds, with A a transition and B a non-transition metal. In particular he discussed d-s bonded hydrides and d-p bonded silicides and carbides in terms of a simple tight binding model (similar to Pettifor's work) which made use of the results of elaborate self-consistent KKR calculations of total energies. The numerical calculations gave results in good agreement with experiment, while the tight-binding model gave a good physical interpretation of the bonding in these compounds.

Experiments on interstitial hydrogen impurities in transition metals were described by Y. Fukai (Chuo Univ., Tokyo). These systems are distinctly different from most substitutional alloys regarding the formation of hydrogen bonding states which are observed by soft x-ray and electron spectroscopy and also NMR measurements. In addition some recent experimental results on the isotope (H or D) dependence of the electrical resistivity and NMR were presented. The isotope effects provide important information regarding the interplay of the conduction electrons and the finite extension of the wave function of an interstitial hydrogen atom.

A theoretical lecture on resistivity "saturation" in transition metals and compounds was given by P.B. Allen (SUNY [State Univ. of New York], Stony Brook). Near room temperature many d-band compounds, notably the high T_c A15's, have large electron-phonon resistivities ($\rho > 80\ \mu\Omega cm$) and correspondingly short electron mean free paths ($\ell \sim 10\text{Å}$). Almost without exception, further increases of ρ with T are inhibited. In other words, the resistivity saturates. Allen ventured that the small value of ℓ and the universality of the effect demand an explanation outside the framework of Bloch-Boltzmann theory (which is valid for large ℓ). Allen further argued that the failure of the approximation of semiclassical dynamics used in the theory is the likely problem, and that the unusual resistivity saturation can be identified with non-classical currents carried by virtual interband transitions. Specific calculations of these effects for the A15's remain to be carried out.

A good number of the contributed papers dealt with elaborate numerical calculations of the properties of disordered alloys. This reflects the very substantial progress made in this area during the last few years. In particular Durham, Gyorffy, Temmerman (Univ. of Bristol, UK) and their collaborators presented calculations of the angle-resolved photoemission spectra of Cu-Ni alloys. They used the multiple-scattering version of the coherent potential approximation (KKRCPA). Comparing with the measured spectra they showed the

effects of alloying in a striking way. They also used the KKRCPA to obtain the local densities of states and the x-ray band spectra in Ag-Pd alloys.

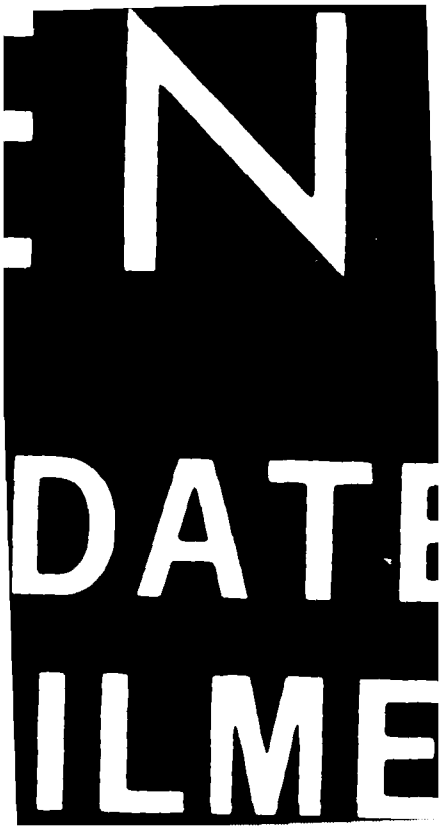
The average t-matrix approximation (ATA) was used by A. Bansil et al (Northeastern Univ.) to calculate the electron momentum density in Cu-Ni alloys. Comparison with positron annihilation experiments was satisfactory.

Klein et al (NRL) used a tight-binding version of the CPA to calculate the electronic properties of the substoichiometric refractory monocarbides NbC_x, TaC_x, and HfC_x.

Rietschel and Winter (Kernforschungscentrum, Karlsruhe) presented an interesting paper in which they argued that depression of superconductivity by spin fluctuations is a widespread phenomenon. They gave results for V, Nb, NV, and V_3Si which appear to be consistent with specific heat and superconductivity measurements.

D. Papaconstantopoulos (NRL) discussed recent theoretical work which explained the variation of T_c with alloying in the materials $NbC_{1-x}N_x$. He showed that the observed maximum in T_c at $x \sim 0.87$ was due to peaking of the electron-phonon interaction at that concentration. Several posters dealt with experiments and interpretations of hydride materials.

Of particular interest was the work of Venema et al (Netherlands) who have observed some interesting isotope dependence of the dHVA spectra of PdH_x and PdD_x ($x \gtrsim 0.0$) possibly due to anomalous zero-point motion of H or D. Stocks and Butler (Oak Ridge) presented ab initio calculations of the residual resistivity of Pd-Ag alloys in remarkably good agreement with experiment. P. Ziesche (Technical Univ., Dresden) presented results of a new band structure method developed by his group using an energy-linearized version of the KKR method. Carbotte's group (McMaster Univ., Ontario, Canada) discussed new solutions to the Eliashberg superconductivity equations which take into account the explicit energy dependence of the electronic density of states. There were a number of experimental papers dealing with spin glasses.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